

Tryptophan, methyl, 2-PFP

Inchi:	InChI=1S/C17H10F10N2O4/c1-33-11(30)10(28-12(31)14(18,19)16(22,23)24)8-6-29(9-5-
InchiKey:	AOAGFUVREFGYJI-UHFFFAOYSA-N
Formula:	C17H10F10N2O4
SMILES:	COC(=O)C(NC(=O)C(F)(F)C(F)(F)F)c1cn(C(=O)C(F)(F)C(F)(F)F)c2ccccc12
Mol. weight [g/mol]:	496.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.53		Crippen Method
logp	4.007		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
rinpol	1855.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R580097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/35-010-1/Tryptophan-methyl-2-PFP.pdf>

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